

# **CHAPTER-10**

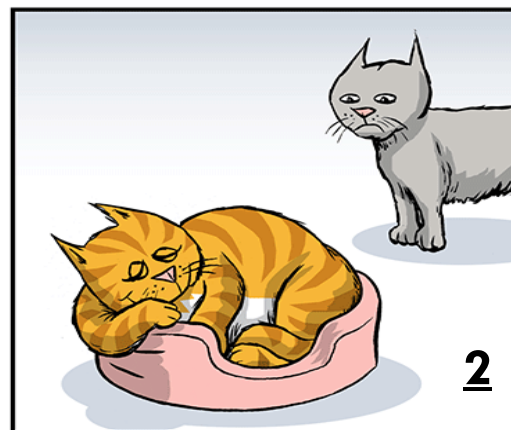
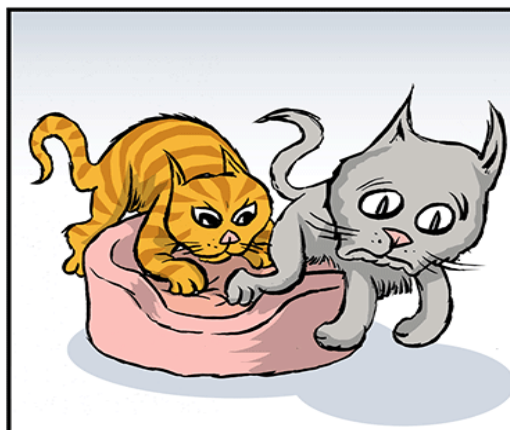
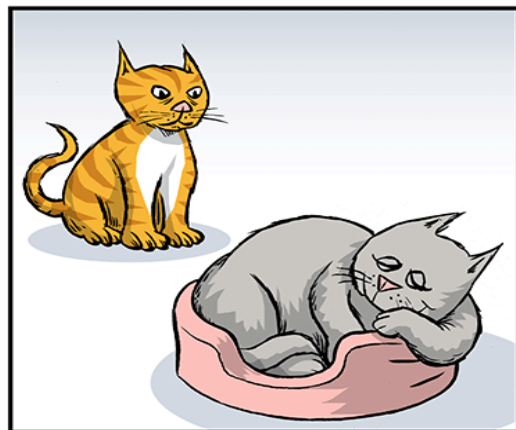
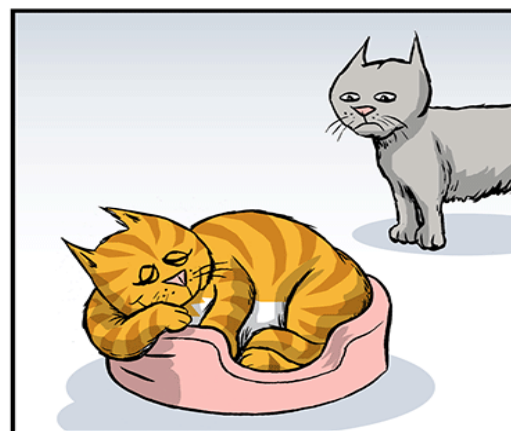
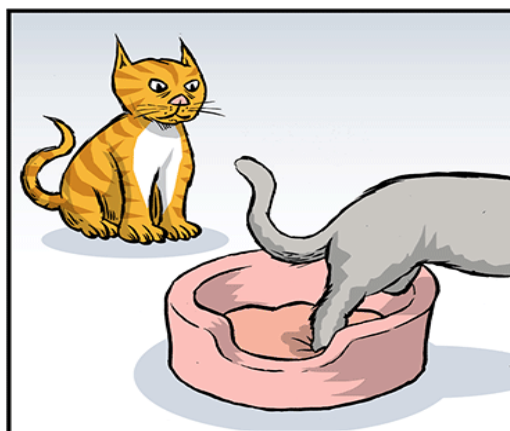
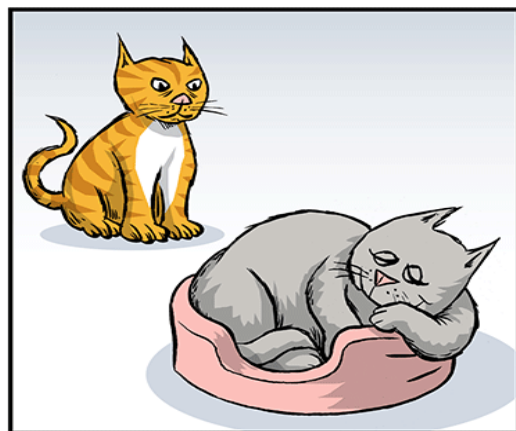
## **CLASS 12**

# **HALOALKANES AND HALOARENES**

### **SUBTOPIC-**

- **REACTION MECHANISM OF SN1 AND SN2**
- **COMPARISON BETWEEN SN1 AND SN2**
- **ROLE OF SOLVENT IN SN1 AND SN2**

# THE CATS AND THE EASY CHAIR CLEARLY EXPLAINS **SN1** AND **SN2** REACTION



# The story of the two cats and the

## Easy chair

Cat 1 finds Cat 2 on his easy chair  
and  
starts to think.

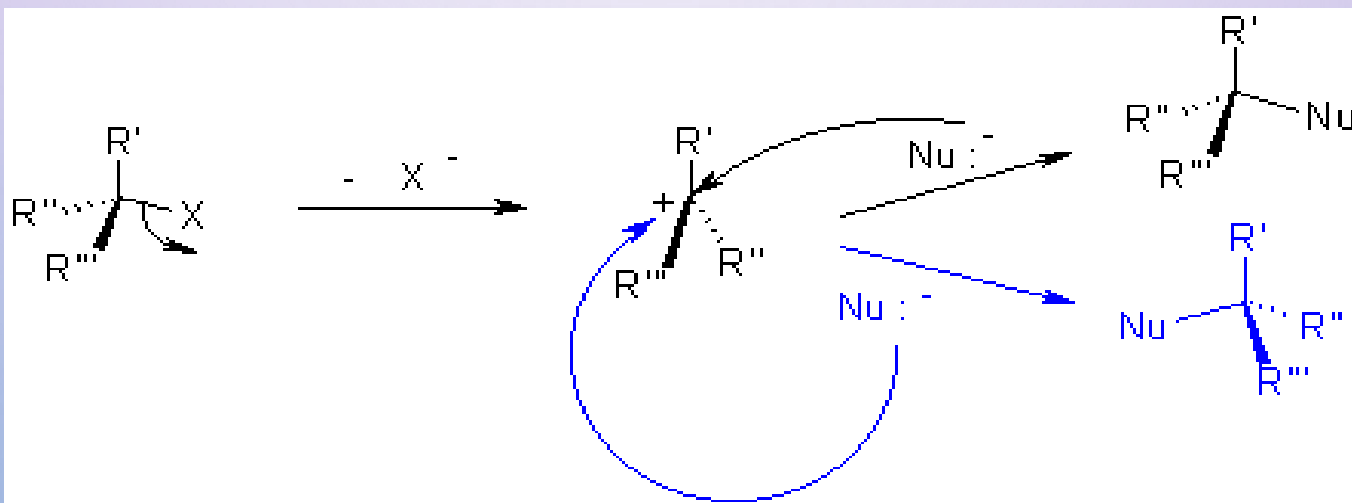
There are two options available to  
the

Cat 1

- He can wait for Cat 2 to leave  
, and then sit in the easy chair.
- He can kick the Cat 2
- out of his easy chair.

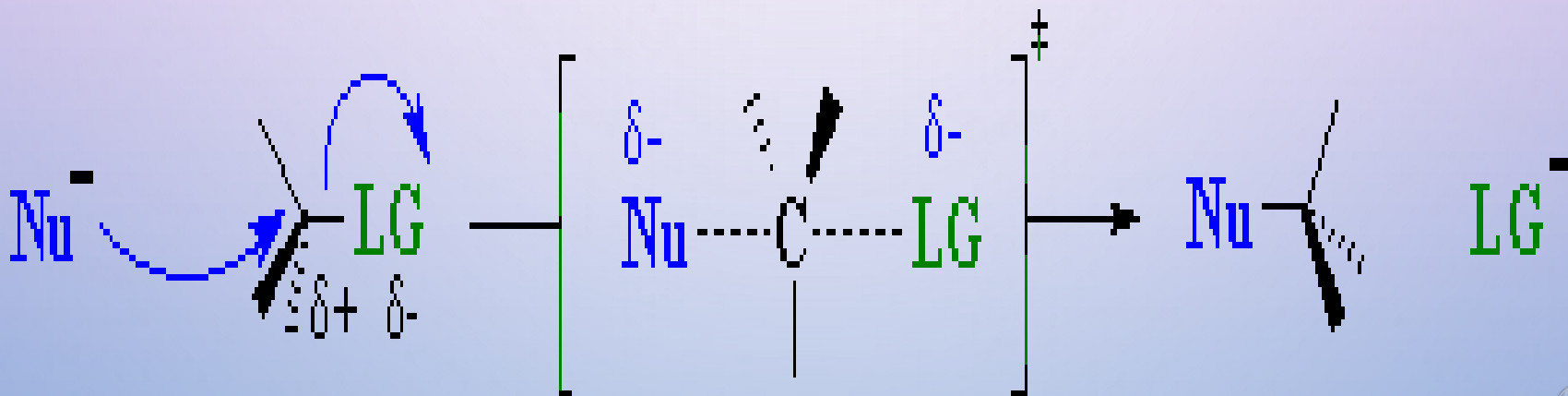
# Mechanism of $S_N1$ reaction

In this reaction a planar carbocation is formed first which then reacts further with the nucleophile. Since the nucleophile is free to attack from either side 50% retention in configuration takes place and 50% inversion in configuration takes place the product formed is called a racemic mixture.



# MECHANISM OF S<sub>N</sub>2 reaction

THE REACTION INVOLVES A BACKSIDE ATTACK OF A NUCLEOPHILE.  
THE REACTION INVOLVES FORMATION OF A TRANSITION STATE WHERE  
THE INCOMING GROUP IS IN THE PROCESS OF FORMING A BOND AND  
THE LEAVING GROUP IS IN THE PROCESS OF LEAVING.  
THE PRODUCT FORMED IS INVERTED ( INVERSION) IN CONFIGURATION  
TAKES PLACE.





# The story of the two Cats

Now I think you can relate the story about the cats and the easy chair with the  $S_N2$  &  $S_N1$

In the  $S_N2$  reaction, the nucleophile (Cat-1) forms a bond with the substrate molecule (easy chair) at the same time when the leaving group (Cat -2) leaves.

In the  $S_N1$  reaction, the leaving group (Cat -2) leaves the substrate (easy chair), and then the nucleophile (Cat -1) forms a bond.

# COMPARISON OF SN1 AND SN2

## • SN1 REACTION

- IT IS SUBSTITUTION NUCLEOPHILIC UNIMOLECULAR REACTION.
- PROCEEDS IN TWO STEPS.
- FIRST STEP IS THE SLOW ONE INVOLVING DISSOCIATION OF THE SUBSTRATE TO FORM CARBOCATION INTERMEDIATE.
- IT IS FAVORED BY POLAR SOLVENTS.
- MOSTLY GIVEN BY TERTIARY ALKYL HALIDES.
- IT OCCURS WITH RACEMIZATION.
- IT FOLLOWS 1ST ORDER KINETICS.
- $\text{RATE} = k[\text{R-X}]$

## • SN2 REACTION

- IT IS SUBSTITUTION NUCLEOPHILIC BIMOLECULAR REACTION.
- PROCEEDS IN A SINGLE STEP WHICH IS THE RATE DETERMINING STEP.
- THE FIRST STEP IS A SLOW STEP AND INVOLVES THE FORMATION OF A TRANSITION STATE.
- IT IS FAVORED BY NON POLAR SOLVENTS.
- MOSTLY GIVEN BY PRIMARY ALKYL HALIDES.
- IT OCCURS WITH 100% INVERSION OF CONFIGURATION.
- IT FOLLOWS 2ND ORDER KINETICS.
- $\text{RATE} = k[\text{R-X}][\text{NU}]$

# THE TYPES OF SOLVENT USED IN NUCLEOPHILIC SUBSTITUTION REACTION

THERE ARE TWO TYPES OF POLAR SOLVENTS; *POLAR PROTIC* AND *POLAR APROTIC*.

POLAR PROTIC SOLVENTS ARE THOSE WHICH CAN MAKE HYDROGEN BONDING I.E. THEY CONTAIN A HYDROGEN CONNECTED TO AN ELECTRONEGATIVE ATOM AND THUS CAN MAKE INTERMOLECULAR HYDROGEN BONDING IN ADDITION TO THE DIPOLE-DIPOLE INTERACTIONS. COMMON POLAR PROTIC SOLVENTS ARE THE WATER AND ALCOHOL.

POLAR APROTIC SOLVENTS, ON THE OTHER HAND, ARE THE ONES WITHOUT A HYDROGEN CONNECTED TO AN ELECTRONEGATIVE ATOM AND THE KEY DIFFERENCE COMPARED TO POLAR PROTIC SOLVENTS IS THE LACK OF INTERMOLECULAR HYDROGEN BONDING.

FOR EX COMMON POLAR APROTIC SOLVENTS ARE ACETONE, ACETONITRILE, DMF AND DMSO



# THE ROLE OF SOLVENT IN UNIMOLECULAR NUCLEOPHILIC SUBSTITUTION REACTION

## S<sub>N</sub>1 & S<sub>N</sub>2

- S<sub>N</sub>1 REACTION PROCEEDS IN THE PRESENCE OF POLAR PROTIC SOLVENTS, SUCH AS WATER AND ALCOHOLS, ORGANIC ACIDS AND INORGANIC ACIDS (H<sub>2</sub>SO<sub>4</sub>, H<sub>3</sub>PO<sub>4</sub>)
- THE POLAR SOLVENTS STABILIZE THE INTERMEDIATE STATE BY SOLVATING THE CARBOCATION AND THEREFORE INCREASE THE RATE OF REACTION.
- POLAR APROTIC SOLVENTS ARE THE SOLVENTS THAT DO NOT HAVE ACIDIC PROTON SUCH AS DMSO, DMF, CH<sub>3</sub>CN, THEY INCREASE THE RATE OF S<sub>N</sub>2 REACTIONS BY SOLVATING THE CATION THUS MAKING THE NUCLEOPHILE MORE AVAILABLE TO REACT.

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